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Analysis of temperature dependence of thermal expansion in $CaSiO_3$ and $(Mg_{1-x}Fe_x)SiO_3$ perovskites

K Y Singh and B R K Gupta*

Department of Physics, G B Pant University of Agriculture and Technology, Pantnagar-263 145, U. S Nagar, Uttaranchal, India

E-mail brkg@rediffmail.com

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Abstract : In the present study, we have calculated the volumes of $CaSiO_3$, $MgSiO_3$, $(Mg_{0.9}Fe_{0.1})SiO_3$ and $(Mg_{0.8}Fe_{0.2})SiO_3$ perovskites under high temperature and high pressures using the Shanker equation of thermal expansivity. The results obtained are found to be in close agreement with the recent experimental P-V-T data for the solids under study. It has been concluded that the Anderson-Gruneisen parameter varies significantly at high temperature and the results are modified. The present method has been found to be useful for predicting the volumes of the solids under high temperatures.

Keywords : Thermal expansion, $(Mg_{1-x}Fe_x)SiO_3$ perovskites, high temperature and pressures

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Recently, Shanker *et al* [1] have derived an equation for thermal expansivity, representing a relationship between volume expansion and temperature, using the method based on the series expansion of lattice potential energy originally due to Born and Huang [2]. In order to understand the thermodynamic and thermoelastic behaviour of solids at high temperatures and high pressures, it is necessary to have reliable values of volume expansion corresponding to high temperature values. We have therefore, made an efforts to predict the volumes for silicate perovskites which play a very sensitive role in analyzing the thermal expansion coefficients, elastic constants and bulk modulus for these solids.

In the present study, we have modified the Shanker's equation [1] in view of the fact that the value of K_0' which is the first pressure derivative of bulk modulus at $P = 0$ can be considered equal to Anderson-Gruneisen parameter δ_T under the assumption that the product of volume thermal expansion coefficient and bulk modulus remain constant at high temperature [3]. Recently, Prasad *et al.* [4] have noted that values of δ_T changes with temperature significantly, whereas in the expression as obtained by Shanker *et al* [1], the values of K_0' have been considered to be constant at all the temperatures. Since the Anderson parameter δ_T and K_0' are the same under the assumption [3], the values of K_0' can not be considered to be a constant parameter at high temperature.

Motivated with this situation, we have thus replaced K_0' by δ_T in the Shanker's expression and made δ_T to be a temperature-dependent, phenomenologically as follows [4] :

$$\delta_T = \delta_T^o (X)^k , \tag{1}$$

where $X = \frac{T}{T_o}$, T_o is the reference temperature (T_o = 300 K) and k is a constant calculated using the relation $k = \left(\frac{\delta \log \delta_T}{\delta \log X}\right)$. Thus, the modified form of Shanker's equation can be written as :

*Corresponding Author

$$\frac{V}{V_o} = \frac{1-\left[1-2/K_o\left\{\left(\delta_T^0(X)^k+1\right)\left(\Delta P_{th}-P\right)\right\}\right]^{\frac{1}{2}}}{\left(\delta_T^o(X)^k+1\right)} \quad (2)$$

where K_o is the value of isothermal bulk modulus and ΔP_{th} is the value of change in thermal pressure which is calculated using the following relationship [5].

$$\Delta P_{th} = \alpha K_T (T - T_o), \quad (3)$$

where α, the thermal expansivity and K_T, the isothermal bulk modulus are the values taken at $P = 0$ and $T = T_o = 300$ K [6]. Above the Debye temperature, the product αK_T becomes nearly constant and the values of ΔP_{th} change linearly with temperature at higher temperatures. The values of V/V_o have been calculated with the help of eq. (2) at selected temperatures and pressures so as to make a direct comparison with the experimental data for silicate perovskites [7–9]. For $CaSiO_3$ perovskite, the thermal pressure has been found virtually independent of volume [7,10] and therefore, the product αK_T remains constant. Hence, we have used the room temperature and zero-pressure value of $\alpha K_T = 7.2 \times 10^{-3}$ GPa/K for $CaSiO_3$ perovskite [7]. For the other three (Mg,Fe) silicate perovskites, we have used $\alpha K_T = 6.92 \times 10^{-3}$ GPa/K determined by Anderson and Masuda [11] by taking the value of α and K_T at $P = 0$ and $T = \theta$, the Debye temperature.

The values used for input parameters in case of $CaSiO_3$ perovskite are taken as $K_o = 232$ GPa, $\delta_T^o = 4.8$ and $V_o = 45.58$ Å. All these values have been determined by Wang *et al* [7] by performing a detailed analysis of their experimental data. They have considered the compatibility with the diamond cell data reported by Mao *et al.*[12] for $CaSiO_3$, to 134 GPa at room temperature. For other three perovskites represented by $(Mg_{1-x}Fe_x)SiO_3$, we take $K_o = 261$ GP_a and $\delta_T^o = 4.1$ as reported by Mao *et al* [8]. It has been found [8] that in case of all three perovskites with $x = 0.0$, 0.1 and 0.2, the room temperature isothermal equations of state are indistinguishable within the uncertaintity limits of the experimental. Using the input data as described above, we have calculated V/V_o with the help of eqs. (2) and (3), for silicate perovskites under simultaneous high pressure and high temperature conditions. The results for $CaSiO_3$ perovskite and $(Mg_{1-x}Fe_x)SiO_3$ perovskites are compared with the experimental data [7,8] in Tables 1 and 2 respectively. We note from the tables that there is good agreement between calculated and experimental values. This implies that the inclusion of phenomenological temperature-dependence of Anderson-Gruneisen parameter determines the results of thermal expansion in solids satisfactorily. On the basis of above discussions and results achieved in the present study, it may thus be concluded that our approach can be employed to the thermal expansions in simple and complex solids at high temperatures and high pressures successfully.

Table 1. Comparison of volumes for $CaSiO_3$ perovskite calculated from equation (2) given in column (a) and experimental values [7] given in column (b).

Temperature (K)	Pressure (GPa)	Volume (Å)^3	
		a	b[7]
301	2.67	45.06	45.03
303	4.10	44.82	44.87
304	9.60	43.90	43.93
306	10.07	43.80	43.83
570	4 70	45.02	45.12
575	9.50	44.21	44.22
770	10.00	44.35	44.38
980	5.50	45.45	45 44
974	7.90	45.01	44.92
976	9.37	44.72	44.71
980	10.50	44.53	44.53
970	11.35	44.40	44 41
1172	11.70	44.57	44.54
	12.02	44.75	44.76

Table 2. Comparison of volumes for $(Mg_{1-x}Fe_x)SiO_3$ perovskites calculated using equation (2) given in column (a) and experimental values [8] given in column (b).

Temperature (K)	Pressure (GPa)	Volume (Å)^3	
		a	b[8]
X - 0.0 300	3.80	160.31	160.46
300	6.30	158.65	158.84
300	13.48	155.29	155.69
X = 0.1 300	2 29	161 29	161.30
300	13.20	155.65	155.70
300	26 00	149.71	149.73
380	26.02	150.09	150.46
544	23.08	151.41	151.63
658	14.18	156.76	156.72
773	10.90	158.24	158.56
877	3.95	163.35	163.72
800	7.50	161.02	161.00
800	9.85	159.25	159.00
700	20.55	153.08	153.17
900	15.50	156.26	156.57
X = 0.2 300	4.80	160.46	160.41
300	13.65	155.79	155.87
300	19.50	153.21	153.37

References

[1] J Shanker, S S Kushwah and P Kumar *Physica* **B233** 78 (1997)

[2] M Born and K Huang *Dynamical Theory of Crystal Lattices* (Oxford : Clarendon) (1954)

[3] J Shanker and M Kumar *Phys. Stat. Sol. (b)* **179** 351 (1993)

[4] A Prasad, M Singh and B R K Gupta *Indian J. Phys.* **76A** 291 (2002)

[5] O L Anderson *Equation of State for Geophysics and Ceramics Science* (Oxford : Oxford University Press) (1995)

[6] S S Kushwah and J Shanker *J. Phys. Chem. Solids* **59** 497 (1998)

[7] Y Wang, D J Weidner and F Guyot *J. Geophys. Res.* **101** 661 (1996)

[8] H K Mao, R J Hemley, Y Fei, J F Shu, L C Chen, A P Jephcoat, Y Wu and W A Bassett *J. Geophys. Res.* **96** 8069 (1991)

[9] N Funamori, T Yagi, W Utsumi, T Kondo, T Uchida and M Funamori *J. Geophys. Res.* **101** 8257 (1996)

[10] O L Anderson *J. Phys. Chem. Solids* **58** 335 (1997)

[11] O L Anderson and K Masuda *Phys. Earth Planet. Inter.* **85** 227 (1994)

[12] H K Mao, L C Chenm, R J Hemley, A P Jephcoat and Y Wu *J. Geophys. Res.* **94** 17889 (1989)